Exercise 1

- Make sure you have an active nanoHUB account – if you do not, please request one – it is free and takes about 3-5 minutes
- Locate and launch the Piece-Wise Constant Potential Barrier Tool on nanoHUB.org
  http://nanoHUB.org/tools/pcpbt
- Explore the out put options for double, triple, and quad barrier structures
- Consider a 2 barrier structure
  - » Increase the barrier heights
    - ✓ Comment on the transmission coefficients and reflection coefficients
    - ✓ Comment on the position of the resonance states
  - » Increase the barrier widths
    - ✓ Comment on transmission coefficents, reflection coefficients and resnonance energie
  - » Do you understand the “bulk bandstructure output”?
    - ✓ Try a set of very tall and thick barriers first. – how do the states compare to a particle in a box calculation

Exercise 2

- Locate and launch the Resonant Tunneling Diode Tool with NEGF on nanoHUB.org
  http://nanoHUB.org/tools/rtdnegf
- Explore the out put options for default values
- Run a Hartree calculation
  - » Comment on the change in charge in the device
  - » Comment on the shape of the current voltage characteristic
  - » Comment on the traces of the eigenenergies
- Turn OFF the relaxation in the reservoirs – turn on Thomas Fermi Potential
  - » Comment on the shape of the I-V

Exercise 3

- Locate and launch the Quantum Dot Lab on nanoHUB.org
  http://nanoHUB.org/tools/qdot
- Explore the out put options for default values
- Select a pyramidal dot
  - » Compare the wave functions in the pyramidal dot to the cubic wavefunctions